

ABSTRACT

A computer system comprises a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of the plurality of chemical compounds on biological systems, a second database containing records corresponding to a plurality of molecular targets, and a third database containing records corresponding to tests of interaction between compounds in the first database and molecular targets in the second database. The tests may include information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target. A user interface is provided to allow a user to view the selected compound and to selectively view information from the first database, the second database, and the third database.

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